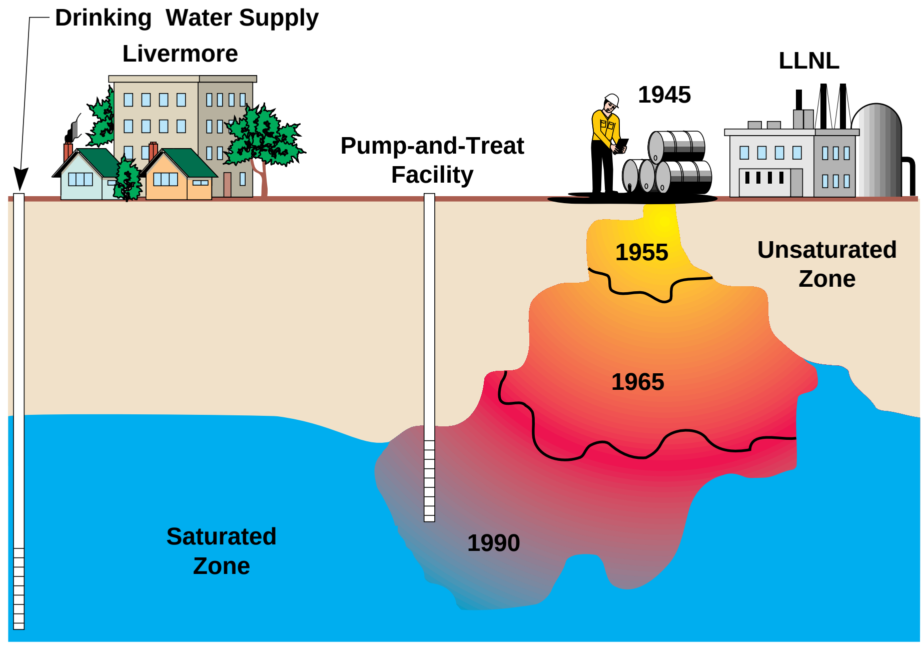
ParFlow

Modeling Subsurface Flow and Chemical Migration on High Perfomance Computers

University of California
Lawrence Livermore National Laboratory

In collaboration with
IT Corporation
Cray Research, Inc.



Contaminants have migrated through the unsaturated zone into the more mobile groundwaters. LLNL is designing and implementing remediation procedures.

Technology

ParFlow is a new simulation code that employs state-of-the-art computational methods and high performance computing technology to enable detailed simulations of fluid flow and chemical transport in three-dimensional, heterogeneous porous media.

Applications

We are using ParFlow to design, manage, and evaluate groundwater remediation and water resource management strategies. Specifically, ParFlow is being used to study the efficacy of pump-and-treat remediation schemes and to help municipalities manage their water supplies more efficiently.

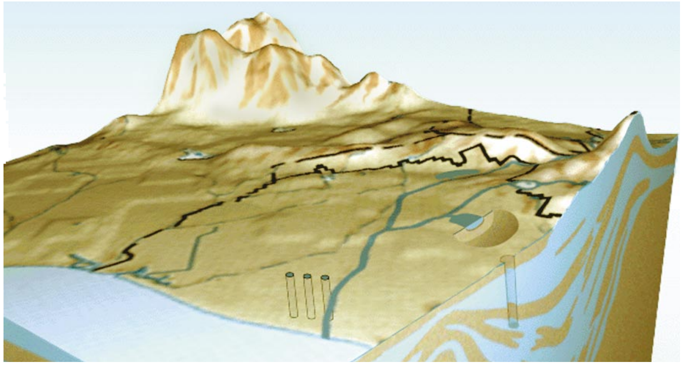
Groundwater remediation and water resource management are major environmental issues throughout the world. In the United States, for instance, numerous governmental and industrial sites, including Lawrence Livermore National Laboratory (LLNL), require remediation. At LLNL, chemical waste products were dumped onto the ground surface in the 1940s when the present site was a naval air station. LLNL is obligated to characterize the contamination and clean it up. Toward this end, various engineered remediation techniques are now being studied, tested, and implemented. Groundwater resource management is a related application of increasing importance, both domestically and internationally: the lack of adequate water supplies of sufficient quality is an impediment to growth in Southern California, and a regional security issue in the Mideast.

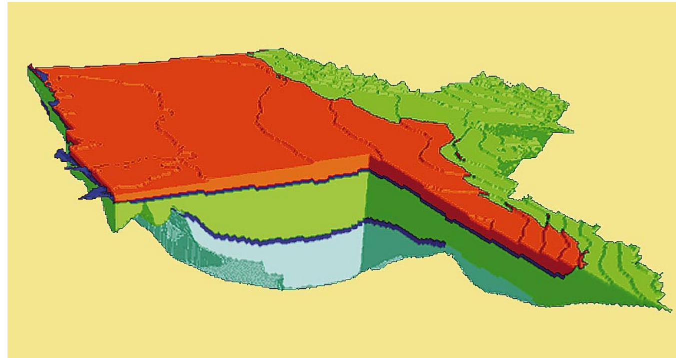
Numerical simulations can be used to determine the most cost-effective cleanup strategy for a contaminated site, as well as to study regional aquifer management issues. Unfortunately, many simulation codes are based on unrealistic assumptions about the subsurface media and its flow behavior. For example, many codes ignore the heterogeneous nature of the subsurface, and instead assume that it is homogeneous. Such codes are incapable of capturing important physical phenomena (such as fingering) that can have a significant impact on fluid flow and contaminant migration. Another flaw of many simulation codes is that they employ outdated and inefficient numerical methods, which preclude running realistic simulations on even the largest conventional vector supercomputers. To compensate for these deficiencies, site managers typically over-engineer the remediation process, which increases costs.

To address this need for an accurate simulation tool, we are developing ParFlow, a sophisticated software package for modeling fluid flow and chemical transport through heterogeneous porous media. To enable detailed simulations of real field sites, ParFlow uses state of the art numerical methods and high-performance computing technologies. These simulations provide site managers with a more realistic picture of contaminant migration, thereby enabling a more cost-effective cleanup strategy. ParFlow also enables large-scale modeling of regional aquifers that encompass hundreds of square miles.

Enabling Large-Scale Simulations

The ParFlow simulator is being used to study groundwater flow and contaminant migration at several sites. The size of these sites (usually





ParFlow is being used to study water resource management issues for the Orange County Water District. An artist's depiction of the Orange County basis is shown on the left; our scalable conceptual model of the area to be modeled is shown on the right.

several square kilometers) and the need to resolve the subsurface heterogeneities (to within a few meters) result in grids with upwards of 100 million spatial zones; similarly sized problems arise in regional aquifer management studies. Since one never has this much hard data about the composition of subsurface materials, we employ geostatistical techniques to generate statistically accurate subsurface realizations from the given field data. This is done in a fully parallel way, starting with a scalable conceptual model of the subsurface (which is defined with the help of the Army's versatile GMS package).

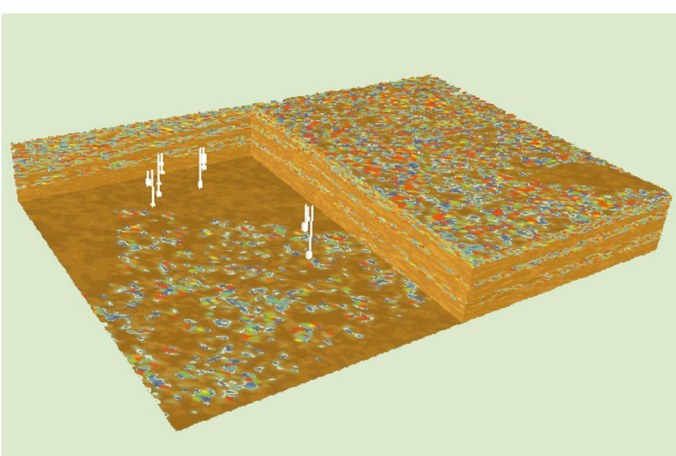
The modeling equations are discretized via finite volumes, and the resulting linear system is solved with a scalable multigrid-preconditioned conjugate gradient algorithm. The resulting flow velocity field is then passed to an advection code to simulate contaminant migration. At present, we have the option of using a particle-in-cell code with reactive chemistry or a grid-based Godunov method.

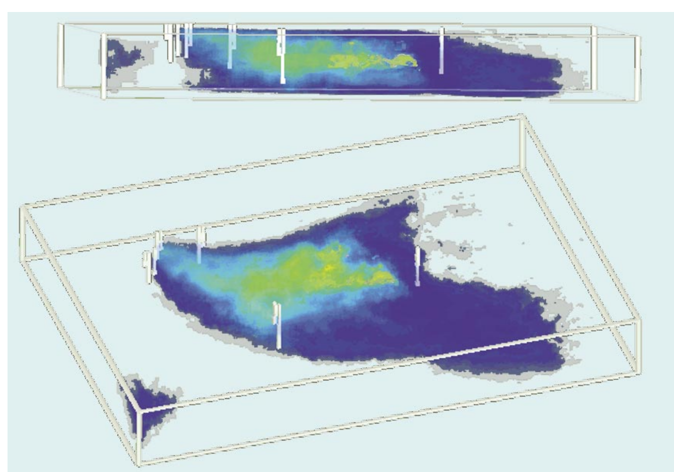
ParFlow is portable across a variety of computing platforms, ranging from workstations to massively parallel computers. Our larger simulations are being run on the Laboratory's CRAY T3D, IBM SP-2, and DEC Alpha cluster. We have demonstrated scalability on several MPP platforms, which means that our code makes efficient use of the additional processors needed for bigger simulations. Our flow solver is especially fast: we have solved realistic flow problems involving eight million spatial zones in just 13 seconds on a 256-processor CRAY T3D.

Multidisciplinary Collaboration

The ParFlow project is a multidisciplinary effort involving scientists from the Center for Applied Scientific Computing and Environmental Programs. LLNL is partnering with IT Corporation and Cray Research, Inc., to commercialize some of aspects of this work.

For additional information about the ParFlow project, contact Steven Ashby, 510-423-2462, sfashby@llnl.gov.





In collaboration with IT Corporation, we are using ParFlow to study various pump-and-treat remediation scenarios for a large industrial site in Northern California. Our scalable conceptual model of the heterogeneous subsurface (with screened pumping wells) is shown on the left. A snapshot in time of a simulation of plume migration is shown on the right.

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